# MONTE CARLO SIMULATION FOR SPHERES WITH TWO LENGTH SCALES

## E.V.R.CHAN

University of Washington
Seattle, Washington, 98195-2420, United States.
evr@u.washington.edu

Canonical ensemble Monte Carlo calculations have been carried out on spheres with two different length scales. Radial distribution functions at various temperatures and densities were computed and compared. Preliminary results indicate that there are differences but because these may be subtle, more calculations including self-diffusion coefficient, heat capacity, etc. would be necessary in order to determine a phase diagram.

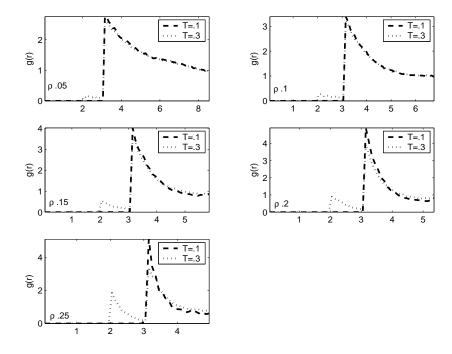


Fig. 1. Radial distribution function g(r) versus radius for densities .05, .1, .15, .2, .25 and temperatures .1 (dashed line) and .3 (dotted line). Density and temperature are in reduced units. At the lower densities the box the particles are enclosed by is bigger and so the radius extends out further at the lower densities.

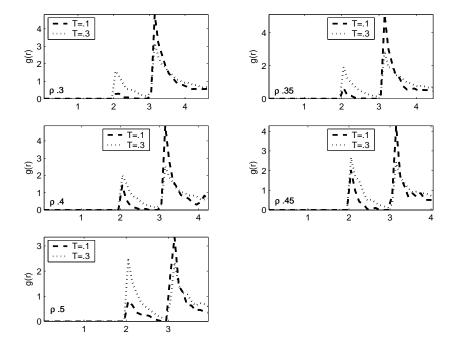


Fig. 2. Radial distribution function g(r) versus radius for densities .3, .35, .4, .45, .5 and temperatures .1 (dashed line) and .3 (dotted line). Density and temperature are in reduced units. At the lower densities the box enclosing the particles is bigger and so the radius extends out further at the lower densities.

## 1. Introduction

Repulsive step potentials, or collapsing spheres<sup>1</sup>, have been used to describe liquidliquid phase transitions<sup>2</sup> and pattern formation in self- organization<sup>3</sup>, The TIP5P model of water<sup>4</sup> has a steep repulsion on the oxygen (part of the Lennard- Jones potential) and Coulombic potentials centered on the hydrogens plus two other points, all tetrahedrally located from the oxygen, so that near the oxygen there is some kind of a step potential.

## 2. Experiment

Simulations using a computer program written to calculate the radial distribution function of hard spheres with a repulsive step were done. The potential is characterized by sigma=2=hard sphere diameter and sigma1=sigma\*1.55=3.1= diameter of second length. The step lies between sigma and sigma1 and has height Ep. For distances greater than sigma1 the potential is zero and less than sigma, is infinite. The temperature used (redT in the program) is in reduced units kT/Ep, where k is the Boltzmann constant.

The reduced density is given by the number of particles divided by the volume

of the box (N/V) and this is multiplied by the hard sphere diameter cubed. The number of particles used is reported<sup>5</sup> to be as low as 32. Recent<sup>6</sup> research indicates that size effects using 32 particles are small. Thirty two particles were used in a canonical (NVT constant) ensemble for this preliminary study. The number of equilibration cycles equalled the number of measurement cycles of 100,000 MC cycles. One MC cycle or one Monte Carlo step per particle (MCS), is the equivalent of the "time" it takes for N particles on the average to have had a chance to change their coordinates. As density increased in Figures 1 and 2, the peaks were getting sharper; this is characteristic of greater order among the particles. Structural changes in the arrangements of the spheres are expected<sup>7</sup> to be exhibited by changes in the radial distribution function.

## 3. Conclusions

Preliminary results indicate that there are changes in g(r) brought about by structural changes, however some of these can be subtle. It is best to get more thermodynamic data including mean square displacement and specific heat in order to determine the phase diagram.

## References

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